

LA-UR-95-- 3148

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

TITLE **A NON-LINEAR ALGEBRAIC MODEL FOR THE
TURBULENT SCALAR FLUXES**

AUTHOR(S) Bassam A. Younis, City University, London
Charles G. Speziale, Boston University
Timothy T. Clark, T-3

SUBMITTED TO *International Conference on Turbulent Heat Transfer, San Diego,
California, March 10-15, 1996*

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy.

Los Alamos

**Los Alamos National Laboratory
Los Alamos, New Mexico 87545**

FORM NO. 836 R4
ST. NO. 2629 5/81

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Interim ICASE Report
and
Draft Paper for
the
International Conference on Turbulent Heat Transfer
San Diego, California
March 10-15, 1996

**A NON-LINEAR ALGEBRAIC MODEL FOR THE
TURBULENT SCALAR FLUXES**

Bassam A. Younis*
Department of Civil Engineering
City University
London EC1V 0HB - UK

Charles G. Speziale
Aerospace and Mechanical Engineering Department
Boston University
Boston, Massachusetts 02215

Timothy T. Clark
Theoretical Division
Theoretical Fluid Dynamics
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

*This research was supported by the National Aeronautics and Space Administration under NASA Contract No. NAS1 - 19480 while the authors were in residence at the Institute for Computer Applications in Science and Engineering (ICASE), NASA Langley Research Center, Hampton, VA 23681-0001.

1 Introduction

The purpose of this paper is to report on a novel approach to the modelling of the turbulent scalar fluxes ($\overline{u_i \theta}$) which arise as a consequence of time averaging the transport equation for a mean scalar (Θ). The focus of this paper will be on the case where Θ is a 'passive' scalar: the extension of this approach to cases involving buoyancy and compressibility will be briefly discussed.

The need for a new approach to modelling the scalar fluxes stems from the lack of realism in the performance of the simple gradient-transport models and the inadequacy of many of the assumptions underlying the more complicated scalar-flux transport closures. The problems with the simple gradient-transport closures are well known. In models of this type, the scalar fluxes are related to the mean scalar field via a scalar turbulent diffusivity (Γ_t), thus:

$$-\overline{u_i \theta} = \Gamma_t \frac{\partial \Theta}{\partial x_i} \quad (1)$$

where, for example:

$$\Gamma_t = \frac{C_\mu k^2}{\sigma_\theta \epsilon} \quad (2)$$

k and ϵ are, respectively, the turbulent kinetic energy and dissipation rate while σ_θ is the appropriate Prandtl-Schmidt number. Models of this type fail badly in complex and strongly-buoyant flows as Eq. (1) is clearly too simplistic in its representation of the scalar fluxes (note, for example, the absence of an explicit dependence on the Reynolds stresses or on the mean shear). Equation (1) also implies that the turbulent diffusivity is isotropic and that the turbulent scalar fluxes and the mean scalar gradients are aligned. Neither result holds true in complex two- and three-dimensional shear flows. Batchelor (1949) proposed a generalization to the gradient-transport hypothesis involving the definition of a turbulent eddy-diffusivity tensor (D_{ij}), thus:

$$-\overline{u_i \theta} = D_{ij} \frac{\partial \Theta}{\partial x_j} \quad (3)$$

Several attempts have been made at obtaining a practical representation for D_{ij} . Some of these (by Yoshizawa (1985,1988), Rogers et al. (1989) and Rubinstein and Barton (1991)) will be discussed later in the paper. At this point, however, it is convenient to mention two such proposals. Daly and Harlow (1970) made D_{ij} directly proportional to the Reynolds stresses, thus:

$$-\overline{u_i \theta} = \text{constant} \times \overline{u_i u_k} \frac{\partial \Theta}{\partial x_k} \quad (4)$$

This model has found widespread due to its relative simplicity and ability to account for the anisotropy of turbulent diffusivity. Launder (1988, 1995) has proposed the "WET" model for the scalar fluxes obtains these quantities as:

$$-\overline{u_i \theta} = \frac{k}{\epsilon} (\beta_1 \overline{u_i u_k} \frac{\partial \Theta}{\partial x_k} + \beta_2 \overline{u_k \theta} \frac{\partial \overline{u_i}}{\partial x_k} + \beta_3 g_i \overline{\theta^2}) \quad (5)$$

Launder's model is unique amongst the existing algebraic closures in (i) being implicit in the scalar fluxes and (ii) not being of the gradient-transport type in that it clearly allows for finite scalar

fluxes in the absence of mean scalar gradients. This is indeed possible in practice but only due to the action of transport by the mean-flow and turbulence: a non-local effect which cannot be catered for within the context of algebraic closures. Few examples of the use of the "WET" model in complex shear flows exist and hence little further can be said about the validity of such formulation.

The alternative route to the gradient-transport hypothesis involves calculating the scalar fluxes directly, either from the solution of modelled differential transport equations in which they are the dependent variables or from simplified algebraic relations derived from these differential equations. The exact equations are of the form:

$$\begin{aligned} \frac{\partial(\overline{u_i \theta})}{\partial t} + \frac{\partial(\overline{U_k u_i \theta})}{\partial x_k} = & - \overline{u_k \theta} \frac{\partial U_i}{\partial x_k} - \overline{u_k u_i} \frac{\partial \theta}{\partial x_k} - \beta g_i \overline{\theta^2} \\ & - (\gamma + \nu) \frac{\partial \theta}{\partial x_k} \frac{\partial u_i}{\partial x_k} \\ & - \frac{\partial}{\partial x_k} \left(\overline{u_k u_i \theta} + \frac{p' \theta}{\rho} \delta_{ik} - \gamma u_i \frac{\partial \theta}{\partial x_k} - \nu \theta \frac{\partial u_i}{\partial x_k} \right) \\ & - \frac{p' \theta}{\rho} \frac{\partial \theta}{\partial x_i} \end{aligned} \quad (6)$$

where β is the volumetric expansion coefficient, γ is molecular diffusivity, ρ is the fluid density, and p' is the fluctuating pressure.

The first three terms on the right-hand-side of Eq. (6) represent, respectively, the rates at which $\overline{u_i \theta}$ is generated by the turbulent interaction with the mean field and by the body forces (buoyancy in this case). These terms are the only ones in Eq. (6) that can be treated exactly; the remainder must first be approximated before the system of equations can be solved for the scalar fluxes. The viscous destruction term (which is zero only in isotropic turbulence) is usually neglected in non-isotropic turbulence as well by invoking the assumption of local isotropy at high turbulence Reynolds numbers. This assumption does not rationally account for the energy cascade to high wave numbers, a process which suggests that some dissipation needs to be present (the DNS results of Rogers et al. (1989) obtained in a fully-developed turbulent channel flow even suggest that this term acts as a *production term* in certain circumstances!). The turbulent-transport term is either neglected (as in conventional Algebraic Stress Model closures) or is modelled via a gradient-transport relation. The last term in Eq. (6), the fluctuating pressure-scalar-gradient correlations, may be viewed as the counterpart of the pressure-strain term in the $\overline{u_i u_j}$ transport equation. It is clearly an important agency which requires careful modelling and it is perhaps here that current scalar-flux-transport models are least well developed. An exact expression for this quantity (derived from the instantaneous equations for the scalar and the i-component of momentum) is given as:

$$\frac{p' \theta}{\rho \partial x_i} = \frac{1}{4\pi} \int \left(\frac{\partial^2 u'_l u'_m}{\partial x_l \partial x_m} \frac{\partial \theta}{\partial x_i} + 2 \frac{\partial U'_l}{\partial x_m} \frac{\partial u'_m}{\partial x_l} \frac{\partial \theta}{\partial x_i} + \frac{\beta g_i}{\Theta'} \frac{\partial \theta}{\partial x_l} \frac{\partial \theta}{\partial x_l} \right) \frac{dV_{ol}}{r} \quad (7)$$

where the primed quantities are evaluated at distance $\mathbf{x} + \mathbf{r}$.

There are three distinct groupings of terms in Eq. (7): one which is associated with purely turbulence interactions (the 'slow' part, $\pi_{ij,1}$), another which involves interactions between the mean

velocity gradients and fluctuating quantities (the 'rapid' part, $\pi_{ij,2}$) and a third which involves the body forces ($\pi_{ij,3}$). Note that the gradients of the mean scalar do not appear explicitly in Eq. (7).

The conventional approach to modelling the integral expression in Eq. (7) has been to model each of its components separately. Thus, Monin (1965), by analogy with Rotta's return-to-isotropy proposal, suggests the model:

$$\pi_{ij,1} = -C_{1\theta} \frac{\epsilon}{k} \overline{u_i \theta} \quad (8)$$

Launder (1975) models the 'rapid' part as:

$$\pi_{ij,2} = -C_{2\theta} P_{i\theta,1} \quad (9)$$

where $P_{i\theta,1} \equiv -\overline{u_k \theta} \frac{\partial \overline{u_i}}{\partial x_k}$.

This, by simple extension to buoyant flows, gives:

$$\pi_{ij,3} = -C_{3\theta} G_{i\theta} \quad (10)$$

where $G_{i\theta} \equiv -\beta g_i \overline{\theta^2}$.

This piece-wise approach to modelling the integral expression (inspired by the once fashionable practice of modelling the equivalent terms in the $\overline{u_i u_j}$ equations, since abandoned; e.g. Speziale et al. 1991) results in the absence from the model of any explicit dependence on terms containing $\overline{u_i u_j}$ and $\frac{\partial \overline{\theta}}{\partial x_k}$. This is a serious omission as the role of the fluctuating pressure-scalar-gradient correlations is to counter-balance the rate of production of $\overline{u_i \theta}$, including that due to the interaction of the Reynolds stresses with the scalar gradients. Interestingly enough, in a DNS study of passive scalar dynamics for fully-developed turbulent channel flow, Rogers et al. (1989) remark that "the results indicate that splitting the pressure term into rapid and slow parts is not a good idea". Jones and Musonge (1987) appear to have been among the first to attempt to restore such dependence. They argued that $\pi_{ij,1}$ and $\pi_{ij,2}$ should be modelled together since both ultimately depend on the mean field. Their proposal reads:

$$\pi_{ij,1} + \pi_{ij,2} = -C_{1\theta} \frac{\overline{u_i \theta}}{\tau} + C_{2\theta} a_{ij} \frac{\partial \overline{\theta}}{\partial x_j} + d_{ijk} \frac{\partial \overline{u_j}}{\partial x_k} \quad (11)$$

where

$$a_{ij} = \left(\frac{\overline{u_i u_j}}{q^2} - \frac{\delta_{ij}}{3} \right)$$

$$\tau = (1 + C'_{1\theta} \sqrt{A_2}) \frac{q^2}{\epsilon}; A_2 = a_{ij} a_{ij}$$

$$d_{ijk} = C_{3\theta} \delta_{ij} \overline{u_k \theta} + C_{4\theta} \delta_{ik} \overline{u_j \theta} + C_{5\theta} \delta_{jk} \overline{u_i \theta}$$

The model is of some complexity and involves six coefficients. A similar result was arrived at by Dakos and Gibson (1987) from the use of Fourier transforms to derive non-linear expressions by

formal solution (in wave-number space) of the Navier-Stokes and the scalar equations. In contrast to these more rigorous approaches, Craft and Launder (1989) (see also Launder, 1995) proposed that $\pi_{ij,1}$ should be modelled as:

$$\pi_{ij,1} = -C_{1\theta} \frac{\epsilon}{k} \left(\overline{u_i \theta} (1 + 0.6 A_2) + C'_{1\theta} a_{ik} + C''_{1\theta} a_{ik} a_{kj} \right) - C'''_{1\theta} Rk a_{ij} \frac{\partial \Theta}{\partial x_j} \quad (12)$$

where $C_{1\theta}$ and $C'''_{1\theta}$ are functions of A_2 and the stress invariant. No explanation was offered, nor is one obvious, for the inclusion of the mean-scalar gradient in a purely turbulence-turbulence interactions term.

It will have become clear from the above that the basis for the modelling of the fluctuating pressure-scalar-gradient term are somewhat precarious. Application to wall-bounded flows introduces further uncertainties in the form of additional terms to account for the effects of a wall in damping the fluctuating pressure field in its vicinity (Gibson and Launder, 1978). These terms involve 'wall damping' functions that limit the model's applicability to simple geometries where such functions can be specified without ambiguity. All in all, therefore, it is reasonable to conclude that while gradient-transport models are inadequate, scalar-flux transport models are defective in their formulation and do not necessarily justify the increased computing overhead required. The motivation is thus clear for the abandonment of both closure strategies in favour of more rationally-derived relations of an algebraic nature.

2 Model Formulation

The proposal we wish to advance through this paper is that an explicit algebraic relation for $\overline{u_i \theta}$ may be constructed, not from the reduction of the transport equation for this quantity (as this will then involve the ill-modelled pressure-fluctuating temperature gradients term), but rather from the utilization of representation theorems based on a rationally assumed functional relationship which is then reduced through the application of appropriate constraints. For an incompressible flow with a passive scalar, the following functional relationship may be assumed:

$$-\overline{u_i \theta} = f_i(\overline{u_i u_j}, S_{ij}, W_{ij}, \Theta_j, \rho, \epsilon, \overline{\theta^2}, \Theta) \quad (13)$$

In the presence of body forces, the relationship would become:

$$-\overline{u_i \theta} = f(\overline{u_i u_j}, S_{ij}, W_{ij}, \Theta_j, \rho, \epsilon, \overline{\theta^2}, \Theta, g_i) \quad (14)$$

In compressible and reacting flows, the following relationship may be appropriate:

$$-\overline{u_i \theta} = f(\overline{u_i u_j}, S_{ij}, W_{ij}, \Theta_j, \rho, \epsilon, \Theta, \overline{\theta^2}, g_i, \frac{\partial P}{\partial x_j}, \frac{\partial \rho}{\partial x_j}, M_t) \quad (15)$$

M_t is the turbulent Mach number.

In the above, S_{ij} and W_{ij} are, respectively, the mean rate of strain and mean vorticity tensors:

$$S_{ij} = \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (16)$$

$$W_{ij} = \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (17)$$

We can introduce ϵ_θ which is the rate of dissipation of the scalar variance $\overline{\theta^2}$. This quantity is related to the dissipation rate of turbulence kinetic energy via the relation:

$$\frac{\epsilon_\theta}{\epsilon} = R^{-1} \frac{0.5\overline{\theta^2}}{0.5\overline{u_i u_i}} \quad (18)$$

and R is the time-scale ratio which is taken as a known constant.

We confine our attention to the incompressible case for which the general representation to the functional relationship of Eq. 13 is:

$$\begin{aligned} -\overline{u_i \theta} = & \alpha_1 \Theta_{,i} + \alpha_2 \tau_{ij} \Theta_{,j} + \alpha_3 S_{ij} \Theta_{,j} + \alpha_4 \tau_{ik} \tau_{kj} \Theta_{,j} + \alpha_5 S_{ik} S_{kj} \Theta_{,j} \\ & + \alpha_6 W_{ij} \Theta_{,j} + \alpha_7 W_{ik} W_{kj} \Theta_{,j} + \alpha_8 (S_{ik} W_{kj} + S_{jk} W_{ki}) \Theta_{,j} \\ & + \alpha_9 (\tau_{ik} S_{kj} + \tau_{jk} S_{ki}) \Theta_{,j} + \alpha_{10} (\tau_{ik} W_{kj} + \tau_{jk} W_{ki}) \Theta_{,j} \\ & + \alpha_{11} g_i + \alpha_{12} \tau_{ij} g_j + \alpha_{13} S_{ij} g_j + \alpha_{14} \tau_{ik} \tau_{kj} g_j + \alpha_{15} S_{ik} S_{kj} g_j \\ & + \alpha_{16} W_{ij} g_j + \alpha_{17} W_{ik} W_{kj} g_j + \alpha_{18} (S_{ik} W_{kj} + S_{jk} W_{ki}) g_j \\ & + \alpha_{19} (\tau_{ik} S_{kj} + \tau_{jk} S_{ki}) g_j + \alpha_{20} (\tau_{ik} W_{kj} + \tau_{jk} W_{ki}) g_j \end{aligned} \quad (19)$$

where

$$\alpha_i = \alpha_i(k, \epsilon, \overline{\theta^2}, \rho, I_\alpha), i = 1, \dots, 20$$

and I_α consists of all possible invariants of the tensor variables listed in Eq. (13).

We may simplify the above by assuming:

1. the anisotropies and turbulent time scales are sufficiently small to allow for a multilinear expansion (the terms containing $\alpha_4, \alpha_5, \alpha_7$ and α_8 are neglected);
2. there is equal balance between the effects of rotational and irrotational strain rates so that they enter through a production-type mechanism only. Thus we have:

$$\alpha_6 = \alpha_3$$

and

$$\alpha_{10} = -\alpha_9$$

The following compact form is then obtained:

$$-\overline{u_i \theta} = \alpha_1 \Theta_{,i} + \alpha_2 \tau_{ij} \Theta_{,j} + \alpha_3 U_{i,j} \Theta_{,j} + \alpha_9 (\tau_{ik} U_{j,k} + \tau_{jk} U_{i,k}) \Theta_{,j} \quad (20)$$

The lengthscale of turbulence is taken to be of the form:

$$l = \frac{k^{\frac{3}{2}}}{\epsilon} \quad (21)$$

Two different timescales are available in flows with scalar transport: the scalar timescale (τ_s) and the dynamic turbulence timescale (τ_d). The ratio of the former to the latter is, of course, the quantity R obtained in Eq. (18). It is legitimate to use either of the two timescales for the purpose of scaling the general representation but, to be consistent with the choice of the turbulence lengthscale, we adopt the dynamic timescale which is given by:

$$\tau_d = \frac{k}{\epsilon} \quad (22)$$

With the above, the algebraic expression for $\overline{u_i \theta}$ in **non-buoyant** flows takes the final form to the lowest order:

$$\begin{aligned} -\overline{u_i \theta} = & C_1 \frac{k^2}{\epsilon} \frac{\partial \Theta}{\partial x_i} \\ & + C_2 \frac{k}{\epsilon} \overline{u_i u_j} \frac{\partial \Theta}{\partial x_j} \\ & + C_3 \frac{k^3}{\epsilon^2} \frac{\partial U_i}{\partial x_j} \frac{\partial \Theta}{\partial x_j} \\ & + C_4 \frac{k^2}{\epsilon^2} \left(\overline{u_i u_k} \frac{\partial U_j}{\partial x_k} + \overline{u_j u_k} \frac{\partial U_i}{\partial x_k} \right) \frac{\partial \Theta}{\partial x_j} \end{aligned} \quad (23)$$

where the C 's are dimensionless constants to be determined by reference to DNS and experimental data.

The first line in the simplified relation corresponds exactly to the simple gradient-transport model given in Eq. (1) when C_1 is set equal to $\frac{C_\mu}{\sigma_\theta}$. The second line is immediately recognizable as the Daly and Harlow model in Eq. (4). Lines 3 and 4 bring in dependencies that are not present in any of the algebraic models reported to date. Their presence here is supported by the outstanding analysis of Dakos and Gibson (1987) who obtained an expression for the fluctuating pressure-scalar-gradient term that contained similar products of mean velocity and scalar gradients.

It is interesting to consider at the very start some of the limiting forms of the new proposal. When a scalar gradient $\frac{\partial \Theta}{\partial y}$ is imposed on an isotropic turbulence field only the scalar-flux component $\overline{v \theta}$ is non-zero and the present relation predicts this quantity as:

$$-\overline{v \theta} = \frac{k^2}{\epsilon} (C_1 + \frac{2}{3} C_2) \frac{\partial \Theta}{\partial y} \quad (24)$$

In non-isotropic turbulence, the imposition of a scalar gradient in a given direction is known to generate scalar fluxes in the directions at right angle to it. Thus, in a two-dimensional flow in the x -direction with mean-velocity U , the imposition of $\frac{\partial \Theta}{\partial y}$ would generate a scalar flux in the streamwise direction ($\overline{u \theta}$). The correct prediction of this flux component is very important in a number of situations, especially in buoyant-flow conditions (e.g. in buoyant plumes where the streamwise flux is the dominant production agency for the turbulence kinetic energy and in the classic cavity flow with one heated and one cooled vertical surfaces). Equation (1) predicts this

quantity as zero but the present proposal gives:

$$-\overline{u\theta} = C_2 \frac{k}{\epsilon} \overline{uv} \frac{\partial \Theta}{\partial y}. \quad (25)$$

In a flow with finite $\frac{\partial \Theta}{\partial y}$, the imposition of a velocity gradient in the same direction may increase or decrease the streamwise scalar flux depending on whether the sign of the velocity gradient is the same or opposite that of the scalar gradient. For this case, the present proposal gives:

$$\begin{aligned} -\overline{u\theta} &= C_2 \frac{k}{\epsilon} \overline{uv} \frac{\partial \Theta}{\partial y} \\ &+ C_3 \frac{k^3}{\epsilon^2} \frac{\partial U}{\partial y} \frac{\partial \Theta}{\partial y} \\ &+ C_4 \frac{k^2}{\epsilon^2} \overline{v^2} \frac{\partial U}{\partial y} \frac{\partial \Theta}{\partial y} \end{aligned} \quad (26)$$

We consider below the relation between the model proposed herein and a number of existing alternatives. Yoshizawa (1985) used the two-scale direct interaction approximation to obtain a diffusion tensor (D_{ij}) which is linear in the velocity gradients. His result, which is valid for arbitrary Reynolds numbers, is given by:

$$D_{ij} = C_1 \frac{k^2}{\epsilon} \delta_{ij} - C_2 \frac{k^3}{\epsilon^2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (27)$$

In a shear flow with finite $\frac{\partial U_j}{\partial x_2}$, this formulation does not permit for the diffusivity components D_{12} and D_{21} to be unequal. This latter defect was absent from the formulation of Rubinstein and Barton (1991), obtained by application of renormalization group theory. At high Reynolds number, their model gives:

$$D_{ij} = C_1 \frac{k^2}{\epsilon} \delta_{ij} - C_2 \frac{k^3}{\epsilon^2} \frac{\partial U_j}{\partial x_i} - C_3 \frac{k^3}{\epsilon^2} \frac{\partial U_i}{\partial x_j} \quad (28)$$

Yoshizawa (1988) made a further proposal, given by:

$$D_{ij} = 4C_k \left(\frac{\overline{\theta^2}}{\epsilon_\theta} \right)^2 \epsilon \delta_{ij} - 8 \left(\frac{\overline{\theta^2}}{\epsilon_\theta} \right)^3 \epsilon \left[C_1 \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + C_1' \left(\frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} \right) \right] \quad (29)$$

None of these models contain an explicit dependence on $\overline{u_i u_j}$, something which is clearly present in the exact equation for $\overline{u_i \theta}$. This dependence was restored in the model of Rogers et al. (1989) who replaced the terms representing the time-change of the scalar fluxes, their dissipation and the fluctuating pressure-scalar-gradient correlations by a multiple of the scalar-flux vector. Their model is given by:

$$\overline{u_i \theta} = -O_{in}^{-1} \overline{u_n u_j} \frac{\partial \Theta}{\partial x_j} \quad (30)$$

where O^{-1} is the reciprocal of the determinant of the tensor O_{ij} which is defined as:

$$O_{ij} = \frac{C_D}{\tau} \delta_{ij} + \frac{\partial U_i}{\partial x_j} \quad (31)$$

where τ is the timescale.

The authors point out that the matrix O_{ij} becomes stiff for values of $S\tau/C_D \gg 1$ but the model suffers a more serious problem; namely, for flows subjected to normal mean strains - such as plane strain or the axisymmetric expansion/contraction - Eq. (30) is not necessarily invertible rendering Eq. (29) singular (see Appendix).

The relationship between the present model and the alternatives can best be seen from Tables 1-4 where various components of the diffusivity tensor (D_{ij}) obtained with those models are presented. The results are for the case where $\frac{\partial u}{\partial y}$ is the only non-zero velocity gradient.

3 Appendix

We consider the performance of the Rogers et al. (1989) model with respect to the case of mean flow plane strain i.e. where:

$$U_{1,1} = -U_{2,2} = S$$

and all other components of $U_{i,j}$ are zero. For this case:

$$\underline{Q} = \begin{bmatrix} \frac{C_D}{\tau} + S & 0 & 0 \\ 0 & \frac{C_D}{\tau} - S & 0 \\ 0 & 0 & \frac{C_D}{\tau} \end{bmatrix} \quad (A1)$$

and, obviously,

$$\underline{Q}^{-1} = \begin{bmatrix} \frac{\tau}{C_D + S\tau} & 0 & 0 \\ 0 & \frac{\tau}{C_D - S\tau} & 0 \\ 0 & 0 & \frac{\tau}{C_D} \end{bmatrix} \quad (A2)$$

So, for arbitrary turbulence

$$\overline{u_1 \theta} = \left(\frac{\tau}{C_D + S\tau} \right) \left(\overline{u_1 u_1} \frac{\partial \theta}{\partial x_1} + \overline{u_1 u_2} \frac{\partial \theta}{\partial x_2} + \overline{u_1 u_3} \frac{\partial \theta}{\partial x_3} \right) \quad (A3)$$

$$\overline{u_2 \theta} = \left(\frac{\tau}{C_D - S\tau} \right) \left(\overline{u_2 u_1} \frac{\partial \theta}{\partial x_1} + \overline{u_2 u_2} \frac{\partial \theta}{\partial x_2} + \overline{u_2 u_3} \frac{\partial \theta}{\partial x_3} \right) \quad (A4)$$

$$\overline{u_3 \theta} = \left(\frac{\tau}{C_D} \right) \left(\overline{u_3 u_1} \frac{\partial \theta}{\partial x_1} + \overline{u_3 u_2} \frac{\partial \theta}{\partial x_2} + \overline{u_3 u_3} \frac{\partial \theta}{\partial x_3} \right) \quad (A5)$$

Clearly, if $C_D = S\tau$, the scalar flux $\overline{u_2 \theta}$ becomes infinite. In the vicinity of $C_D \approx S\tau$, the result will be unphysical. For any general irrotational mean flow strain, this model would suffer from similar defects.

Table 1. Models results for diffusivity-tensor component D_{11}

Model	
<i>Present</i>	$C_1 \frac{k^2}{\epsilon} + C_2 \frac{k}{\epsilon} \overline{u^2} + 2C_4 \frac{k^2}{\epsilon^2} \overline{uv} \frac{\partial U}{\partial y}$
<i>Yoshizawa (1985)</i>	$C_1 \frac{k^2}{\epsilon}$
<i>Yoshizawa (1988)</i>	$4C_k \left(\frac{\overline{\theta^2}}{\epsilon_\theta} \right)^2 \epsilon$
<i>Rogers et al. (1989)</i>	$\frac{1}{C_D} \frac{k}{\epsilon} \overline{u^2} - \frac{1}{C_D^2} \frac{k^2}{\epsilon^2} \overline{uv} \frac{\partial U}{\partial y}$
<i>Rubinstein and Barton (1991)</i>	$C_1 \frac{k^2}{\epsilon}$

Table 2. Models results for diffusivity-tensor component D_{22}

Model	
<i>Present</i>	$C_1 \frac{k^2}{\epsilon} + C_2 \frac{k}{\epsilon} \overline{v^2}$
<i>Yoshizawa (1985)</i>	$C_1 \frac{k^2}{\epsilon}$
<i>Yoshizawa (1988)</i>	$4C_k \left(\frac{\overline{\theta^2}}{\epsilon_\theta} \right)^2 \epsilon$
<i>Rogers et al. (1989)</i>	$\frac{1}{C_D} \frac{k}{\epsilon} \overline{v^2}$
<i>Rubinstein and Barton (1991)</i>	$C_1 \frac{k^2}{\epsilon}$

Table 3. Models results for diffusivity-tensor component D_{12}

Model	
<i>Present</i>	$C_2 \frac{k}{\epsilon} \overline{uv} + C_3 \frac{k^3}{\epsilon^2} \frac{\partial U}{\partial y} + C_4 \frac{k^2}{\epsilon^2} \overline{v^2} \frac{\partial U}{\partial y}$
<i>Yoshizawa (1985)</i>	$-C \frac{k^3}{\epsilon^2} \frac{\partial U}{\partial y}$
<i>Yoshizawa (1988)</i>	$-8 \left(\frac{\overline{\theta^2}}{\epsilon_\theta} \right)^3 \epsilon (C_1 + C_1') \frac{\partial U}{\partial y}$
<i>Rogers et al. (1989)</i>	$\frac{1}{C_D} \frac{k}{\epsilon} \overline{uv} - \frac{1}{C_D^2} \frac{k^2}{\epsilon^2} \overline{v^2} \frac{\partial U}{\partial y}$
<i>Rubinstein and Barton (1991)</i>	$-0.076 \frac{k^3}{\epsilon^2} \frac{\partial U}{\partial y}$

Table 4. Models results for diffusivity-tensor component D_{21}

Model	
<i>Present</i>	$C_2 \frac{k}{\epsilon} \overline{uv} + C_4 \frac{k^2}{\epsilon^2} \overline{v^2} \frac{\partial U}{\partial y}$
<i>Yoshizawa (1985)</i>	$-C \frac{k^3}{\epsilon^2} \frac{\partial U}{\partial y}$
<i>Yoshizawa (1988)</i>	$-8 \left(\frac{\overline{\theta^2}}{\epsilon_\theta} \right)^3 \epsilon (C_1 - C_1') \frac{\partial U}{\partial y}$
<i>Rogers et al. (1989)</i>	$\frac{1}{C_D} \frac{k}{\epsilon} \overline{uv}$
<i>Rubinstein and Barton (1991)</i>	$-0.166 \frac{k^3}{\epsilon^2} \frac{\partial U}{\partial y}$

4 References

- Batchelor, G K 1949 Diffusion in a field of homogeneous turbulence. *Austral. J. Sci. Res.* **A2**, pp 437-450.
- Craft, T J and Launder, B E 1989 A new model for the pressure/scalar-gradient correlation and its application to homogeneous and inhomogeneous free shear flows. *Proc. 7th Symp. Turbulent Shear Flows*, Stanford Univ., 17.1.1-17.1.6.
- Dakos, T and Gibson, M M 1987 On modelling the pressure terms of the scalar flux equations. In *Turbulent Shear Flows 5* (ed.), pp. 7-18. Springer.
- Daly, B J and Harlow, F H 1970 Transport equations of turbulence. *Phys. Fluids* **13**, 2634.
- Gibson, M M and Launder, B E 1978 Ground effects on pressure fluctuations in the atmospheric boundary layer. *J. Fluid Mech.* **86**, 491.
- Jones, W P and Musonge, P 1983 Modelling of scalar transport in homogeneous turbulent flow. *Proc. 4th Symp. Turbulent Shear Flows*, Karlsruhe Univ., 17.18-17.24.
- Jones, W P and Musonge, P 1987 Closure of the Reynolds stress and scalar flux equations
- Kaltenbach, h -J, Gerz, T and Schumann, U 1994 Large-eddy simulation of homogeneous turbulence and diffusion in stably stratified shear flow. *J. Fluid Mech.* **280**, 1-40.
- Launder, B E 1978 Heat and mass transport. In *Turbulence* (ed. P. Bradshaw), Topics in Applied Physics, vol. 12, pp. 231-287. Springer.
- Launder, B E 1994 Turbulence modelling for industrial flows. *ICASE/LaRC Short Course*.
- Monin, AS 1965 On the symmetry of turbulence in the surface layer of air. *IZV Atmos. Oceanic Phys.* **1**, pp. 45-54.
- Rogers, M M, Mansour, N N and Reynolds, W C 1989 An algebraic model for the turbulent flux of a passive scalar. *J. Fluid Mech.* **203**, 77-101.
- Rubinstein, R and Barton, J 1991 Renormalization group analysis of anisotropic diffusion in turbulent shear flows. *Phys. Fluids A* **3**, 415-421.
- Speziale, C G 1987 On non-linear k-l and k- ϵ models of turbulence. *J. Fluid Mech.* **178**, 459.
- Speziale, C G, Sarkar, S and Gatski T B 1990 Modelling the pressure-strain correlation of turbulence, an invariant dynamical systems approach. *J. Fluid Mech.* **227**, pp. 245-272.

Sreenivasan, K R, Tavoularis, S and Corrsin, S 1981. A test of gradient transport and its generalisations. In *Turbulent Shear Flows 3* (ed. L J S Bradbury, F Durst, B E Launder, F W Schmidt and J H Whitelaw), pp. 96-112. Springer.

Yoshizawa, A 1985 Statistical analysis of the anisotropy of scalar diffusion in turbulent shear flows. *Phys. Fluids* **28**, 3226-3231.

Yoshizawa, A 1988 Statistical modelling of passive-scalar diffusion in turbulent shear flows. *J. Fluid Mech.* **195**, pp. 541-555.

NTIS does not permit return of items for credit or refund. A replacement will be provided if an error is made in filling your order, if the item was received in damaged condition, or if the item is defective.

Reproduced by NTIS
National Technical Information Service
U.S. Department of Commerce
Springfield, VA 22161

This report was printed specifically for your order from our collection of more than 2 million technical reports.

For economy and efficiency, NTIS does not maintain stock of its vast collection of technical reports. Rather, most documents are printed for each order. Your copy is the best possible reproduction available from our master archive. If you have any questions concerning this document or any order you placed with NTIS, please call our Customer Services Department at (703)487-4660.

Always think of NTIS when you want:

- Access to the technical, scientific, and engineering results generated by the ongoing multibillion dollar R&D program of the U.S. Government.
- R&D results from Japan, West Germany, Great Britain, and some 20 other countries, most of it reported in English.

NTIS also operates two centers that can provide you with valuable information:

- The Federal Computer Products Center - offers software and datafiles produced by Federal agencies.
- The Center for the Utilization of Federal Technology - gives you access to the best of Federal technologies and laboratory resources.

For more information about NTIS, send for our FREE *NTIS Products and Services Catalog* which describes how you can access this U.S. and foreign Government technology. Call (703)487-4650 or send this sheet to NTIS, U.S. Department of Commerce, Springfield, VA 22161. Ask for catalog, PR-827.

Name _____
Address _____

Telephone _____

*- Your Source to U.S. and Foreign Government
Research and Technology.*

